General Physics

THEORETICAL STUDY OF THE VIBRATIONAL MODES IN THE S4 SEGMENT OF A POTASSIUM CHANNEL MOLECULE

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Abstract

The potassium channel molecule of the *Drosophila melanogaster* fruit fly *Shaker* is a voltage-gated molecule. Charged amino acids in the S4 segment of the channel molecule cause the S4 segment to act as a voltage sensor. We have computationally modeled the mechanical vibrations of the S4 segment during activation assuming an alpha helical structure for the entire segment. Nearest and next-nearest neighbor interactions were considered along with stabilizing hydrogen bonds between every four amino acids in the S4 sequence. Channel activation was simulated by rotationally and longitudinally displacing the S4 amino acids from equilibrium. Vibrational modes result due to harmonic restoring forces representing the chemical bonds. The effect of bond strength on vibrational modes will be discussed in terms of energy availability.